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A Posteriori Error Estimators for Solutions to the Time Domain Maxwell Equations

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Review of Maxwell's Equations

- Maxwell's Equations

$$\epsilon\frac{\partial \mathbf{E}}{\partial t}=\nabla\times\mathbf{H}-\mathbf{J},\qquad \nabla\bullet\mathbf{D}=0,\qquad \mathbf{D}=\epsilon\mathbf{E}$$

$$\mu\frac{\partial \mathbf{H}}{\partial t}=-\nabla\times\mathbf{E},\qquad \nabla\bullet\mathbf{B}=0,\qquad \mathbf{B}=\mu\mathbf{H}$$

- Wave Equation

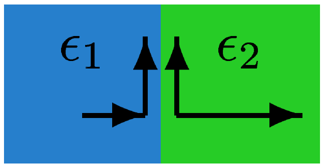
$$\epsilon\frac{\partial^2 \mathbf{E}}{\partial t^2}=-\nabla\times\mu^{-1}\nabla\times\mathbf{E}-\frac{\partial \mathbf{J}}{\partial t}$$

- Diffusion Equation
  - assume $\sigma\mathbf{E}=\mathbf{J}+\epsilon\frac{\partial \mathbf{E}}{\partial t}$

$$\sigma\frac{\partial \mathbf{E}}{\partial t}=-\nabla\times\mu^{-1}\nabla\times\mathbf{E}$$

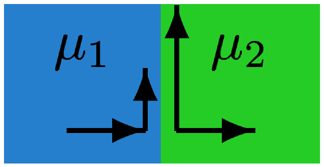
Continuity Considerations

Electric Field ($\mathbf{E}$)



$$\hat{n}\times(\mathbf{E}_1-\mathbf{E}_2)=0,\hat{n}\cdot(\mathbf{D}_1-\mathbf{D}_2)=0$$

Magnetic Flux ($\mathbf{B}$)

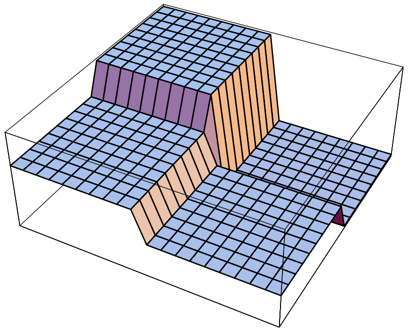


$$\hat{n}\times(\mathbf{H}_1-\mathbf{H}_2)=0,\hat{n}\cdot(\mathbf{B}_1-\mathbf{B}_2)=0$$

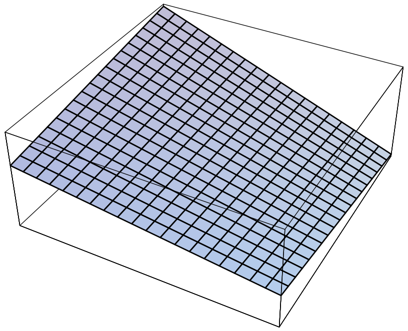
Review of Patch Recovery Error Estimators

- In standard computational elasticity the primary variable is the displacement u. A linear u gives rise to a piecewise constant stress σ.
- Smoothing σ (computing nodal averages) gives a more palatable result to the user, and can be shown to be more accurate (Oden & Reddy, 1973.)
- The smooth (recovered) stress σ_r can be used to estimate the error in the computation (Zienkiewicz & Zhu, 1992,1993.)

Piecewise constant stress σ



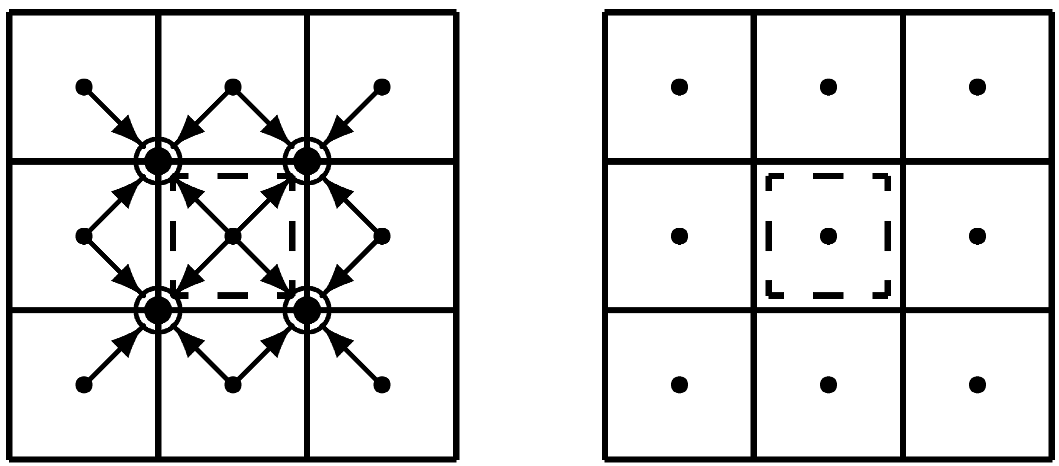
Recovered stress σ_r



$$Error \approx |\sigma_r - \sigma|$$

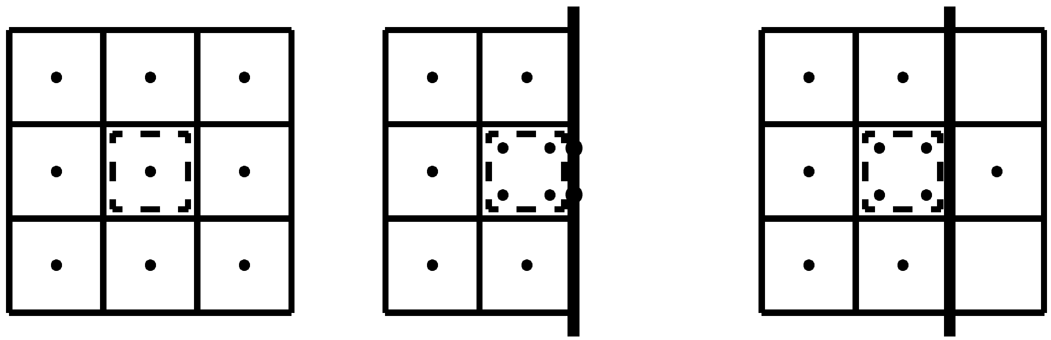
Modified Patch Recovery for Maxwell's Equations

- Modification required
  - We want to process $\mathbf{E}$ and $\mathbf{B}$ directly, not the gradients
  - We need to deal with partial continuity of $\mathbf{E}$ and $\mathbf{B}$
  - Cell-centered vs. node-centered

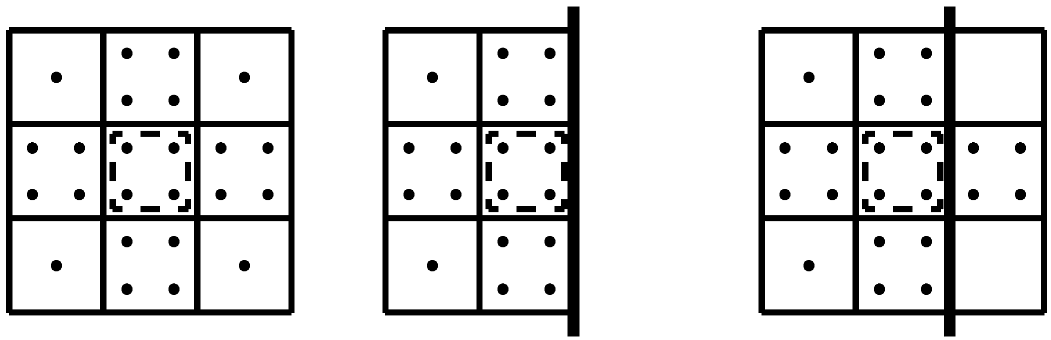


Sampling Points for Modified Patch Recovery

- $\boldsymbol{p = 1}$ Biquadratic polynomial fit



- $\boldsymbol{p = 2}$ Bicubic polynomial fit



Review of Explicit Residual Error Estimators

- For equations of the form:

$$\alpha \nabla \times \chi \nabla \times \mathbf{u}_n + \beta \mathbf{u}_n = \mathbf{f}(\mathbf{j}, \mathbf{u}_{n-1}, \ldots)$$

- The error, $\mathbf{e} := \mathbf{u}(t_n) - \mathbf{u}_n$, satisfies the defect equation:

$$\alpha(\chi \nabla \times \mathbf{e}, \nabla \times \mathbf{q})_{L^2(\Omega)} + (\beta \mathbf{e}, \mathbf{q})_{L^2(\Omega)} = r(\mathbf{q}) \; \forall \mathbf{q} \in H_0(\text{curl})$$

- Definition of the Residual:

$$r(\mathbf{q}) := (\mathbf{f}, \mathbf{q})_{L^2(\Omega)} - \alpha(\chi \nabla \times \mathbf{u}_n, \nabla \times \mathbf{q})_{L^2(\Omega)} - (\beta \mathbf{u}_n, \mathbf{q})_{L^2(\Omega)} \; \forall \mathbf{q} \in H_0(\text{curl})$$

- Explicit Residual methods attempt to measure how closely a computed solution satisfies the differential equation.

- For an analysis of this method for Nédélec's edge elements see Beck, Hiptmair, Hoppe, and Wohlmuth, 2000

Explicit Residual Error Estimators for Maxwell's Equations

- Estimate consists of four separate terms

$$\nabla\cdot\mathbf{D}=0 \quad \rightleftharpoons \quad \eta_0^T:=h_T\|\tfrac{1}{\sqrt{\beta}}\nabla\cdot(\mathbf{f}-\beta\tilde{\mathbf{u}})\|_{L^2(T)}, \quad T\in\mathcal{T}_h$$

$$\hat{n}\cdot(\mathbf{D}_1-\mathbf{D}_2)=0 \quad \rightleftharpoons \quad \eta_0^F:=h_F^{1/2}\|\tfrac{1}{\sqrt{\beta_A}}[\langle\mathbf{n},\mathbf{f}-\beta\tilde{\mathbf{u}}\rangle]_J\|_{L^2(F)}, \quad F\in\mathcal{F}_h$$

$$\text{Diff. Eqn.} \quad \rightleftharpoons \quad \eta_1^T:=h_T\ \|\tfrac{1}{\sqrt{\chi}}(\mathbf{f}-\alpha\nabla\times\chi\nabla\times\tilde{\mathbf{u}}-\beta\tilde{\mathbf{u}})\|_{L^2(T)}, \quad T\in\mathcal{T}_h$$

$$\hat{n}\times(\mathbf{H}_1-\mathbf{H}_2)=0 \quad \rightleftharpoons \quad \eta_1^F:=h_F^{1/2}\|\tfrac{\alpha}{\sqrt{\chi_A}}[\mathbf{n}\times\chi\nabla\times\tilde{\mathbf{u}}]_J\|_{L^2(F)}, \quad F\in\mathcal{F}_h$$

Where

$[\langle\mathbf{n},\mathbf{q}\rangle]_J:=\langle\mathbf{n},\mathbf{q}\rangle_{|F\subset T_{out}}-\langle\mathbf{n},\mathbf{q}\rangle_{|F\subset T_{in}}$ and $[\mathbf{n}\times\mathbf{q}]_J:=\mathbf{n}\times\mathbf{q}_{|F\subset T_{out}}-\mathbf{n}\times\mathbf{q}_{|F\subset T_{in}}$

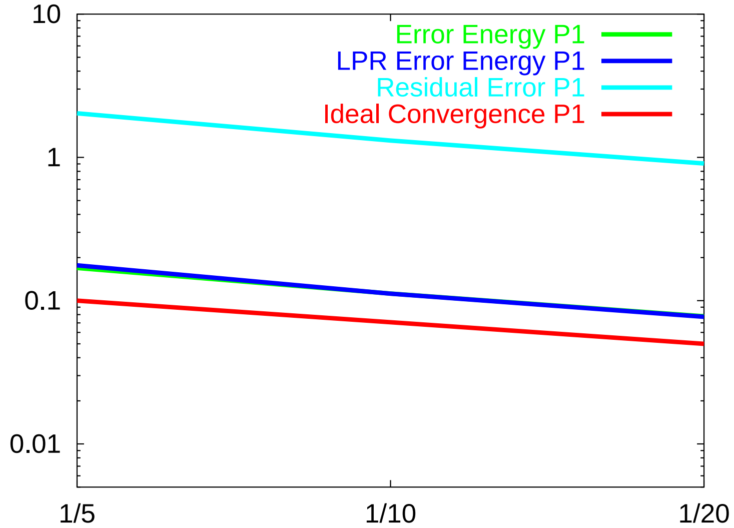
- The total error estimate is given by:

$$\eta_T^2:=(\eta_0^T)^2+(\eta_1^T)^2+\sum_{F\in\mathcal{F}(T)\cap\mathcal{F}^{int}}\frac{\beta_{|T}}{2\beta_A}(\eta_0^F)^2+\frac{\chi_{|T}}{2\chi_A}(\eta_1^F)^2$$

Key Differences of the Two Methods

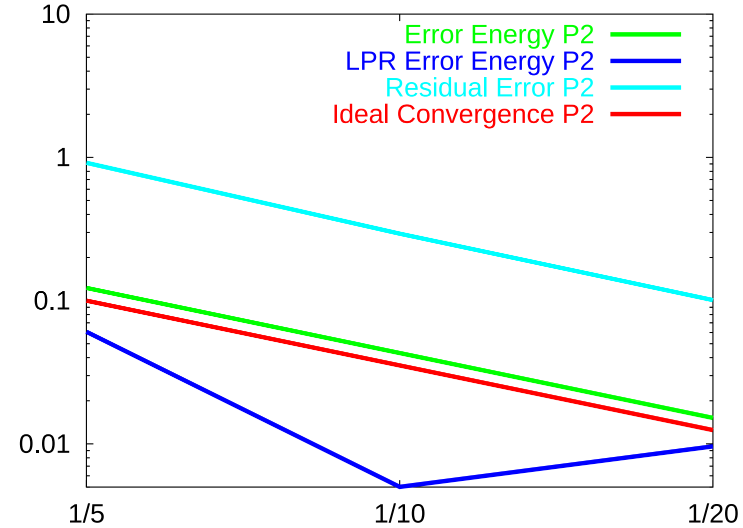
- Residual Methods
  - Not simply a measure of the curvature of the fields
  - Depends on both the field and its derivative
  - Takes into account the specific PDE being solved
  - Takes into account time integration
  - Can distinguish different types of errors
- Patch Recovery
  - Provides a smoother representation of the field
  - Computationally efficient

Convergence Results for the Diffusion Equation on a Distorted Mesh



$$p = 1$$

- True error and LPR overlap
- All measures converge at expected rate

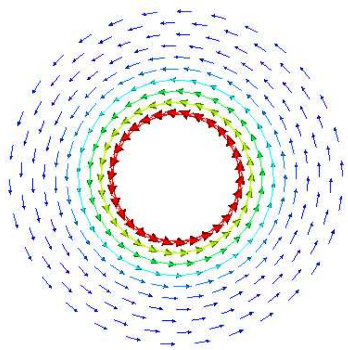


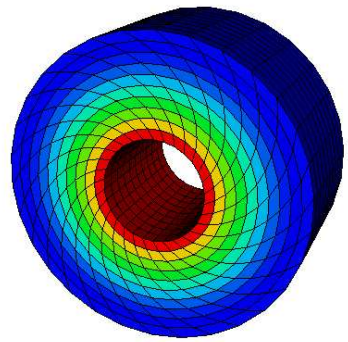
$$p = 2$$

- LPR is rather erratic
- Others converge at expected rate

Error Distribution Results for the Diffusion Equation

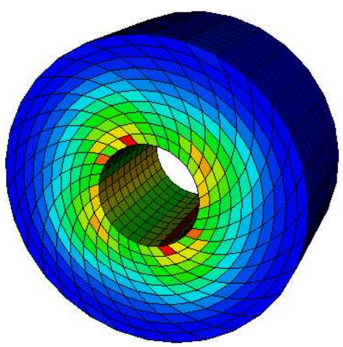
H
Field

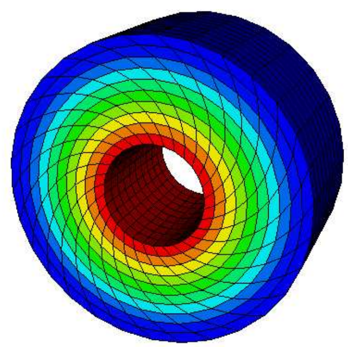




Error
Energy

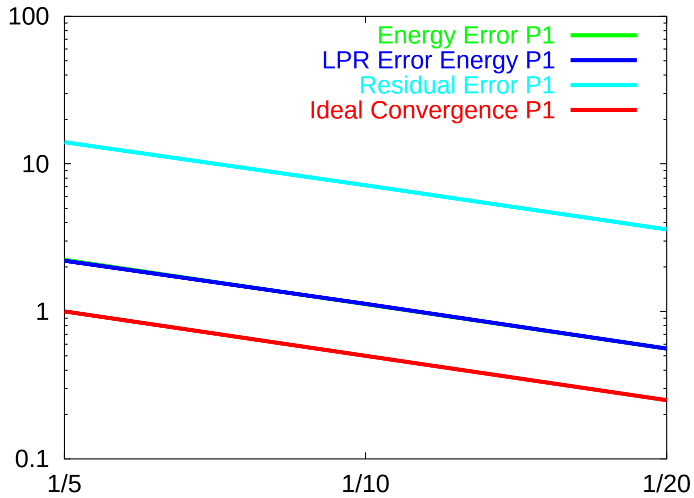
LPR
Error



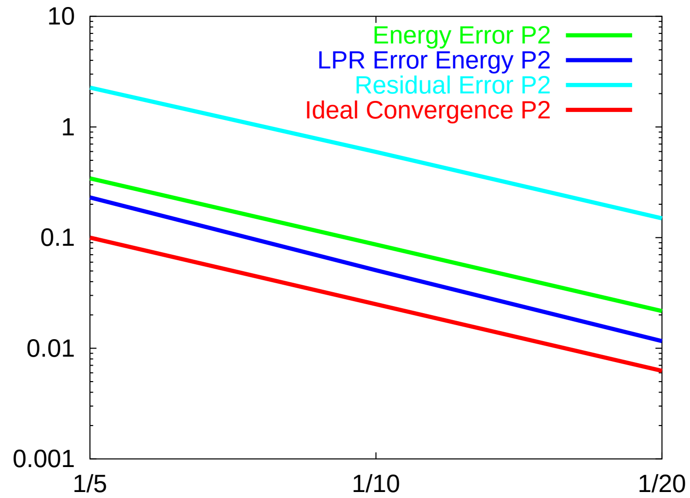


Residual
Error

Convergence Results for the Wave Equation on a Cartesian Mesh



$p = 1$



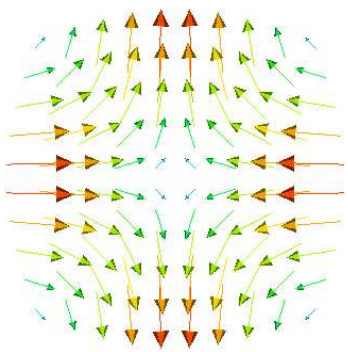
$p = 2$

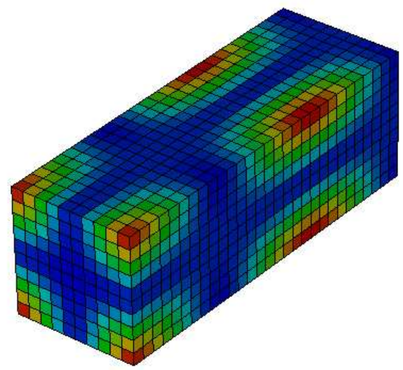
- All errors show expected convergence rate (h^1)
- LPR matches global error but differs spacially

- All errors show expected convergence rate (h^2)
- LPR under-estimates the error

Error Distribution Results for the Wave Equation

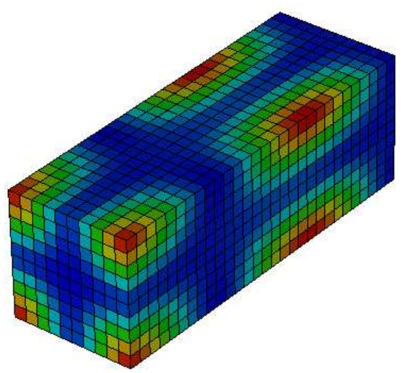
E
Field

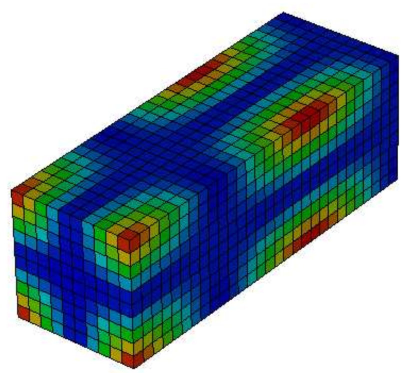




Error
Energy

LPR
Error





Residual
Error

Summary

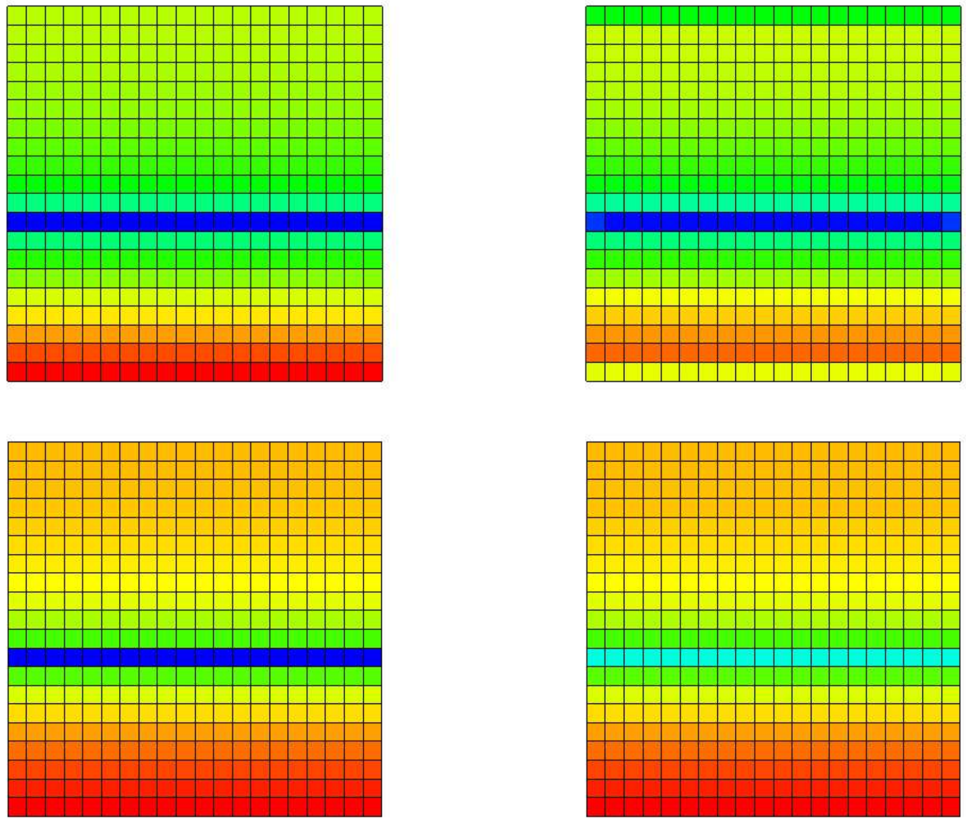
- We developed and tested a modified patch recovery scheme for Maxwell's Equations
  - Computationally efficient
  - Provides a smoothed representation of the solution
- We implemented the Beck-Hiptmair-Hoppe-Wohlmuth explicit residual error estimator concept for both the wave equation and the diffusion equation
  - Works equally well throughout the mesh
  - Distinguishes errors arising from various characteristics of the solution
- Both methods…
  - account for jump discontinuity of fields across material interfaces
  - work for arbitrary order basis functions

Questions...

Error Distribution Results for the Diffusion Equation on a Cartesian Mesh

$\|u-\tilde{u}\|_{L^2}^2$

$\|\nabla\times(u-\tilde{u})\|_{L^2}^2$



LPR Error

Residual Error

Residual Based Error Estimation

$$\alpha \nabla \times \chi \nabla \times \mathbf{u}_n + \beta \mathbf{u}_n = \mathbf{f}$$

Where $\mathbf{u}$ is the new iterative solution computed at a given time step and $\mathbf{f}$ contains both the source term as well as the previous solutions.

- Vector Diffusion Equation for the Electric Field

$$\alpha{=}1/2, \chi{=}\mu^{-1}, \beta{=}\sigma/dt$$

$$\mathbf{f}{=}{-}\partial_t \mathbf{J}{-}(1{-}\alpha)\nabla{\times}\mu^{-1}\nabla{\times}\mathbf{u}_{n-1}{+}\tfrac{\sigma}{dt}\mathbf{u}_{n-1}$$

- Newmark Beta Scheme for the Second order Vector Wave Equation

$$\alpha{=}[0{,}1], \chi{=}\mu^{-1}, \beta{=}\epsilon/dt^2$$

$$\mathbf{f}{=}{-}\partial_t \mathbf{J}{-}\nabla{\times}\mu^{-1}\nabla{\times}\{(1{-}2\alpha)\mathbf{u}_{n-1}{+}\alpha\mathbf{u}_{n-2}\}{+}\tfrac{\epsilon}{dt^2}(2\mathbf{u}_{n-1}{-}\mathbf{u}_{n-2})$$

Definition of The Residual

$$r(\mathbf{q}) := (\mathbf{f}, \mathbf{q})_{L^2(\Omega)} - \alpha(\chi \nabla \times \tilde{\mathbf{u}}, \nabla \times \mathbf{q})_{L^2(\Omega)} - (\beta \tilde{\mathbf{u}}, \mathbf{q})_{L^2(\Omega)} \forall \mathbf{q} \in H_0(\text{curl})$$

Using $\mathbf{e} := \mathbf{u} - \tilde{\mathbf{u}}$ this definition becomes:

$$r(\mathbf{q}) = \alpha(\chi \nabla \times \mathbf{e}, \nabla \times \mathbf{q})_{L^2(\Omega)} + (\beta \mathbf{e}, \mathbf{q})_{L^2(\Omega)} \qquad \forall \mathbf{q} \in H_0(\text{curl})$$

Which we then split in two pieces:

$$\begin{aligned} r(\mathbf{q}^0) &= (\beta \mathbf{e}^0, \mathbf{q}^0)_{L^2(\Omega)} && \forall \mathbf{q}^0 \in H_0^0(\text{curl}) \\ r(\mathbf{q}^\perp) &= \alpha(\chi \nabla \times \mathbf{e}^\perp, \nabla \times \mathbf{q}^\perp)_{L^2(\Omega)} + (\beta \mathbf{e}^\perp, \mathbf{q}^\perp)_{L^2(\Omega)} && \forall \mathbf{q}^\perp \in H_0^\perp(\text{curl}) \end{aligned}$$

$$H_0^0(\text{curl}) := \{\mathbf{q} \in H_0(\text{curl}) | \nabla \times \mathbf{q} = 0\}$$

$$H_0^\perp(\text{curl}) := \{\mathbf{q} \in H_0(\text{curl}) | (\beta \mathbf{q}, \mathbf{q}^0)_{L^2(\Omega)} = 0 \ \forall \mathbf{q}^0 \in H_0^0(\text{curl})\}$$

Resulting Error Terms

- Estimate consists of four separate terms

$$
\begin{array}{llll}
\nabla\cdot\mathbf{D}=0 & \rightleftharpoons & \eta_0^T := h_T \| \frac{1}{\sqrt{\beta}} \nabla\cdot(\mathbf{f}-\beta\tilde{\mathbf{u}}) \|_{L^2(T)}, & T\in\mathcal{T}_h \\
\hat{n}\cdot(\mathbf{D}_1-\mathbf{D}_2)=0 & \rightleftharpoons & \eta_0^F := h_F^{1/2} \| \frac{1}{\sqrt{\beta_A}} [\langle \mathbf{n},\mathbf{f}-\beta\tilde{\mathbf{u}}\rangle]_J \|_{L^2(F)}, & F\in\mathcal{F}_h \\
\text{Diff. Eqn.} & \rightleftharpoons & \eta_1^T := h_T \ \| \frac{1}{\sqrt{\chi}} (\mathbf{f}-\alpha\nabla\times\chi\nabla\times\tilde{\mathbf{u}}-\beta\tilde{\mathbf{u}}) \|_{L^2(T)}, & T\in\mathcal{T}_h \\
\hat{n}\times(\mathbf{H}_1-\mathbf{H}_2)=0 & \rightleftharpoons & \eta_1^F := h_F^{1/2} \| \frac{\alpha}{\sqrt{\chi_A}} [\mathbf{n}\times\chi\nabla\times\tilde{\mathbf{u}}]_J \|_{L^2(F)}, & F\in\mathcal{F}_h
\end{array}
$$

Where

$[\langle \mathbf{n},\mathbf{q}\rangle]_J := \langle \mathbf{n},\mathbf{q}\rangle_{|F\subset T_{out}} - \langle \mathbf{n},\mathbf{q}\rangle_{|F\subset T_{in}}$ and $[\mathbf{n}\times\mathbf{q}]_J := \mathbf{n}\times\mathbf{q}_{|F\subset T_{out}} - \mathbf{n}\times\mathbf{q}_{|F\subset T_{in}}$

- The total error estimate is given by:

$$\eta_T^2 := (\eta_0^T)^2 + (\eta_1^T)^2 + \sum_{F\in\mathcal{F}(T)\cap\mathcal{F}^{int}} \frac{\beta_{|T}}{2\beta_A} (\eta_0^F)^2 + \frac{\chi_{|T}}{2\chi_A} (\eta_1^F)^2$$